



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 PM UTC

PDB ID : 2FNF / pdb_00002fnf
Title : C1 domain of Nore1
Authors : Harjes, E.; Harjes, S.; Wohlgemuth, S.; Krieger, E.; Herrmann, C.; Muller, K.H.; Bayer, P.
Deposited on : 2006-01-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

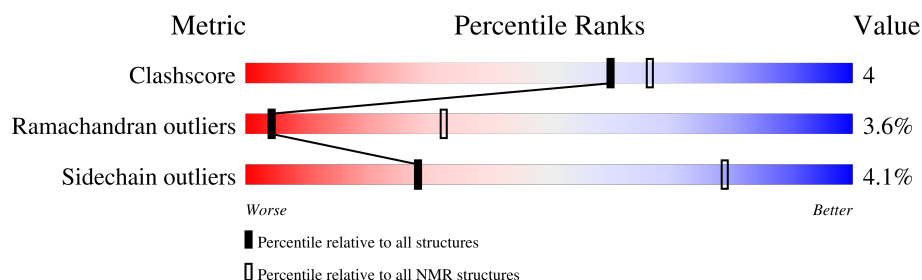
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	X	72	

2 Ensemble composition and analysis

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	X:118-X:123, X:129-X:166 (44)	0.62	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 10, 12, 13, 15, 16, 17, 21, 22, 23, 24, 25, 27, 28, 29, 30
2	11, 14, 19, 26
3	18, 20
Single-model clusters	9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 922 atoms, of which 456 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called putative Ras Effector Nore1.

Mol	Chain	Residues	Atoms							Trace
1	X	59	Total	C	H	N	O	S		0
			920	282	456	95	80	7		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

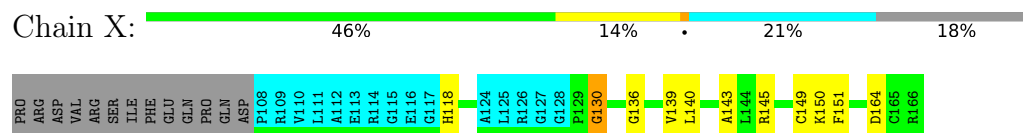
Mol	Chain	Residues	Atoms	
2	X	2	Total	Zn
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: putative Ras Effector Nore1

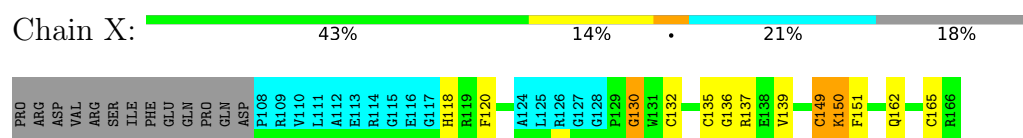


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

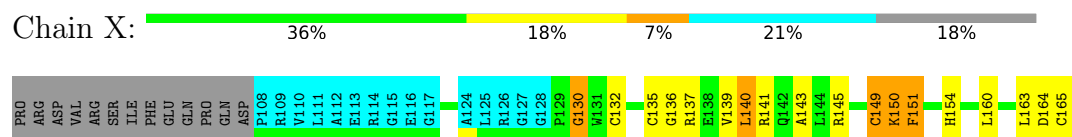
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: putative Ras Effector Nore1



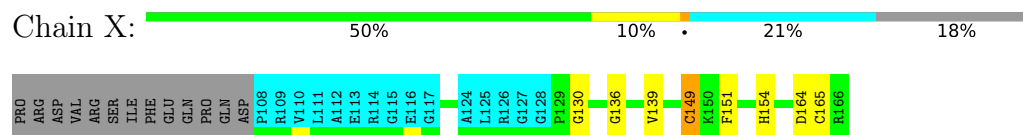
4.2.2 Score per residue for model 2

- Molecule 1: putative Ras Effector Nore1



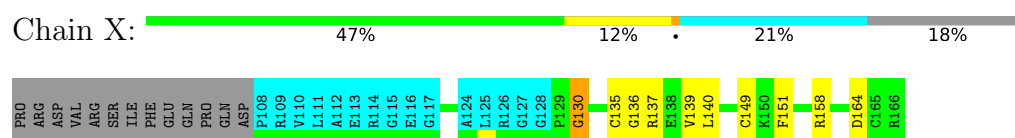
4.2.3 Score per residue for model 3

- Molecule 1: putative Ras Effector Norel



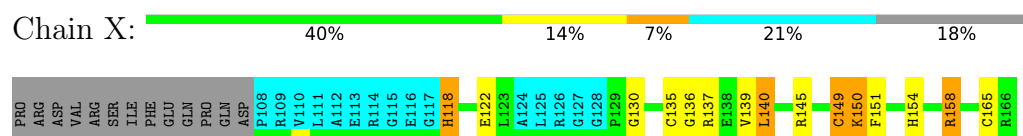
4.2.4 Score per residue for model 4

- Molecule 1: putative Ras Effector Norel



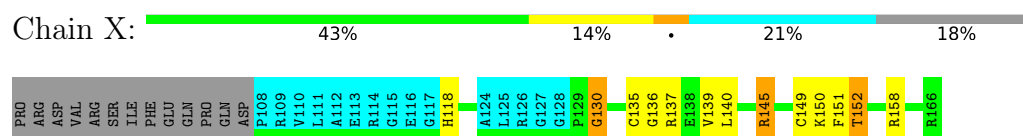
4.2.5 Score per residue for model 5

- Molecule 1: putative Ras Effector Norel



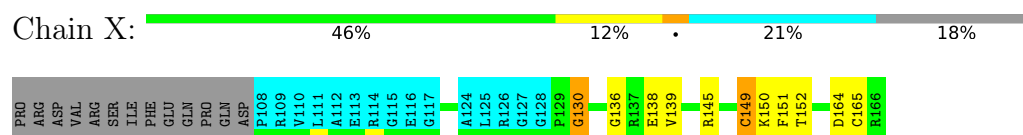
4.2.6 Score per residue for model 6

- Molecule 1: putative Ras Effector Norel



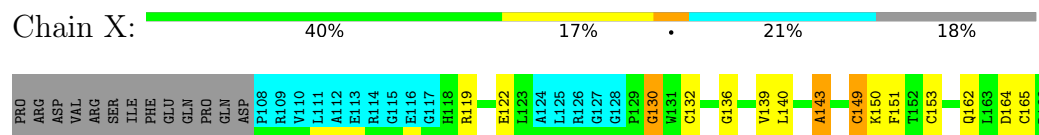
4.2.7 Score per residue for model 7

- Molecule 1: putative Ras Effector Norel



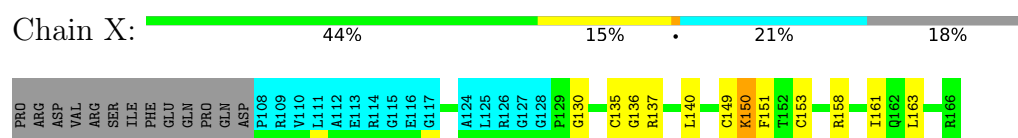
4.2.8 Score per residue for model 8

- Molecule 1: putative Ras Effector Norel



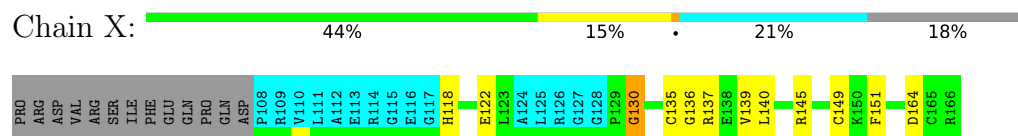
4.2.9 Score per residue for model 9

- Molecule 1: putative Ras Effector Norel



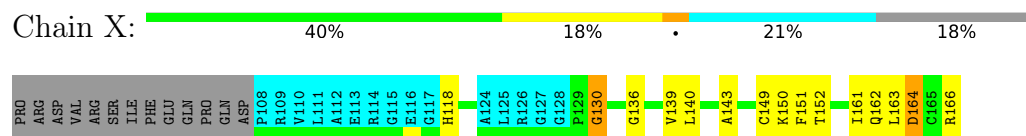
4.2.10 Score per residue for model 10

- Molecule 1: putative Ras Effector Norel



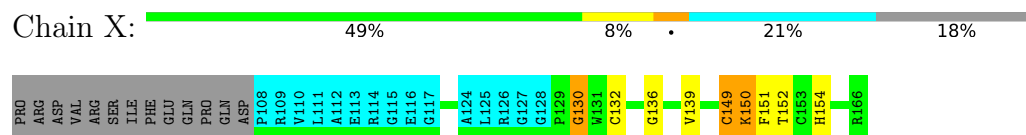
4.2.11 Score per residue for model 11

- Molecule 1: putative Ras Effector Norel



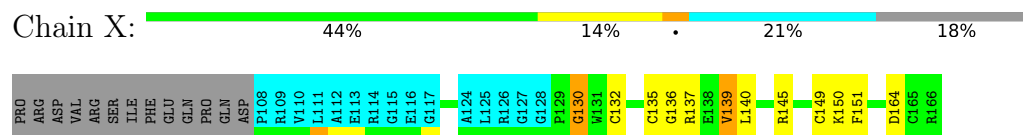
4.2.12 Score per residue for model 12

- Molecule 1: putative Ras Effector Norel



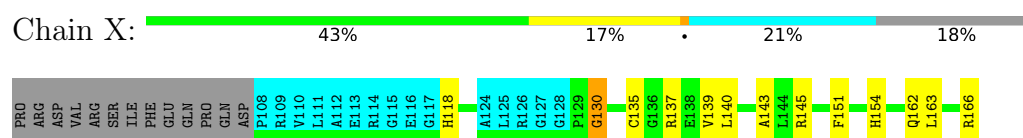
4.2.13 Score per residue for model 13

- Molecule 1: putative Ras Effector Norel



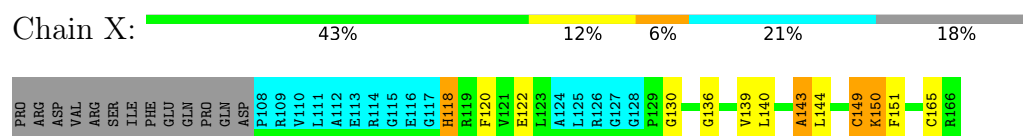
4.2.14 Score per residue for model 14

- Molecule 1: putative Ras Effector Norel



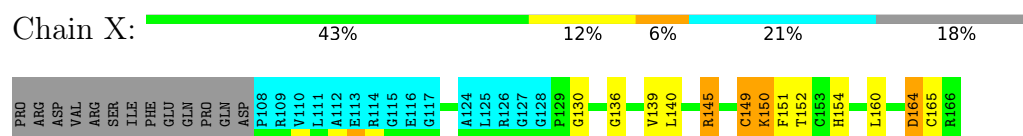
4.2.15 Score per residue for model 15

- Molecule 1: putative Ras Effector Norel



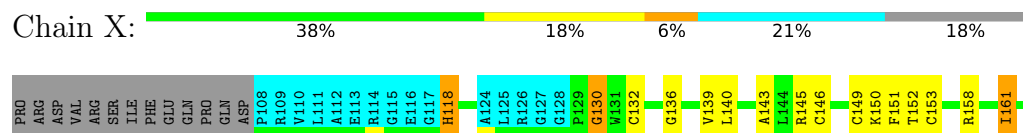
4.2.16 Score per residue for model 16

- Molecule 1: putative Ras Effector Norel



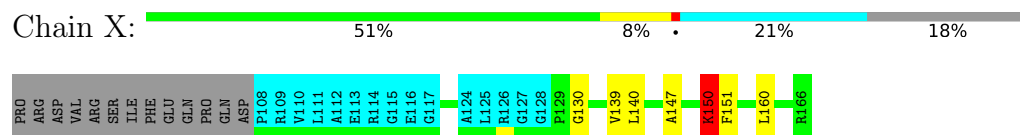
4.2.17 Score per residue for model 17

- Molecule 1: putative Ras Effector Norel



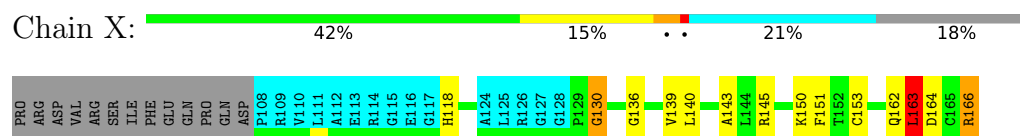
4.2.18 Score per residue for model 18

- Molecule 1: putative Ras Effector Norel



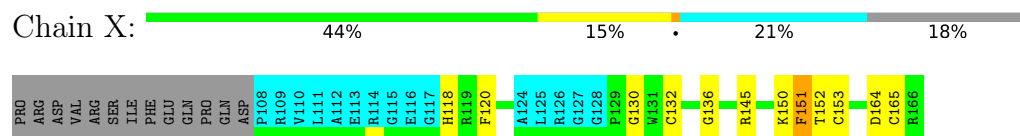
4.2.19 Score per residue for model 19

- Molecule 1: putative Ras Effector Norel



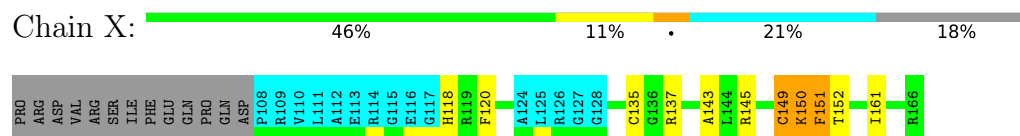
4.2.20 Score per residue for model 20

- Molecule 1: putative Ras Effector Norel



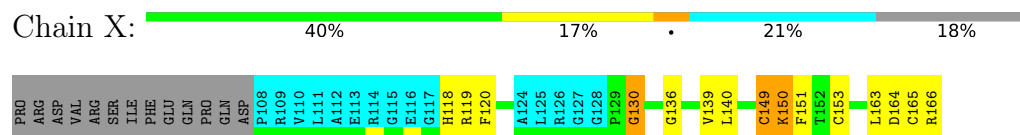
4.2.21 Score per residue for model 21

- Molecule 1: putative Ras Effector Norel



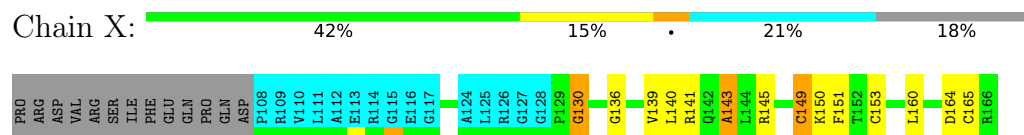
4.2.22 Score per residue for model 22

- Molecule 1: putative Ras Effector Norel



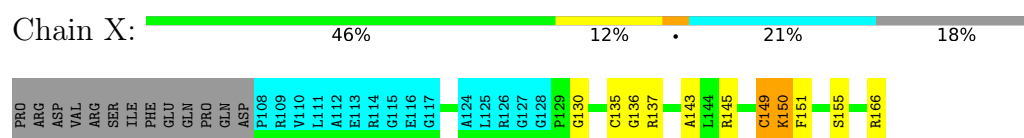
4.2.23 Score per residue for model 23

- Molecule 1: putative Ras Effector Norel



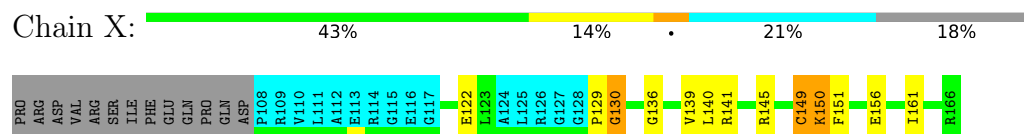
4.2.24 Score per residue for model 24

- Molecule 1: putative Ras Effector Norel



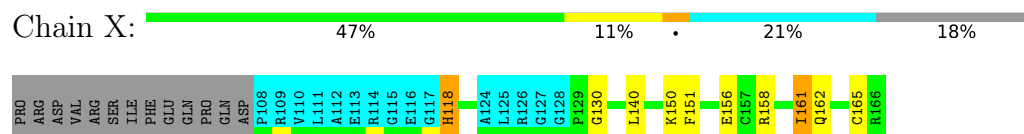
4.2.25 Score per residue for model 25

- Molecule 1: putative Ras Effector Norel



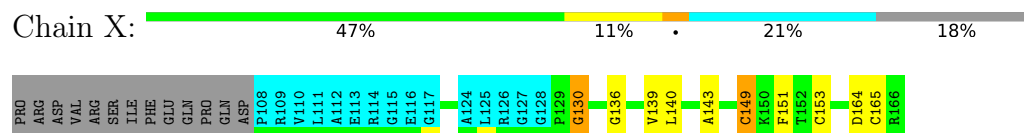
4.2.26 Score per residue for model 26

- Molecule 1: putative Ras Effector Norel



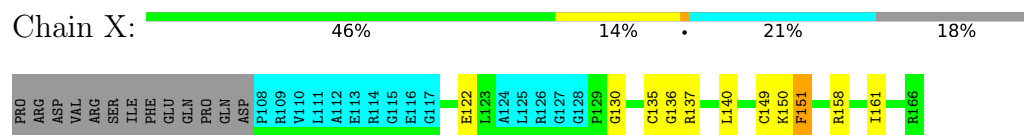
4.2.27 Score per residue for model 27

- Molecule 1: putative Ras Effector Norel



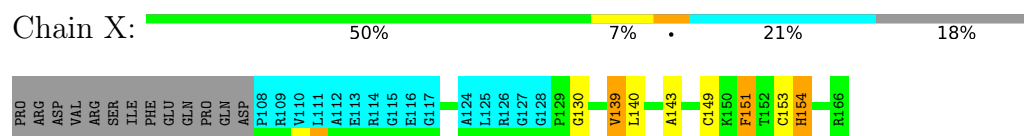
4.2.28 Score per residue for model 28

- Molecule 1: putative Ras Effector Norel



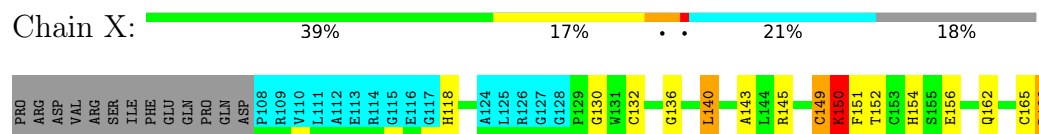
4.2.29 Score per residue for model 29

- Molecule 1: putative Ras Effector Norel



4.2.30 Score per residue for model 30

- Molecule 1: putative Ras Effector Norel



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing; molecular dynamics; torsion angle dynamics*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
YASARA	structure solution	5.11.29
YASARA	refinement	5.11.29

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	X	0.95±0.05	0±1/363 (0.1± 0.2%)	1.52±0.08	6±2/484 (1.3± 0.4%)
All	All	0.96	13/10890 (0.1%)	1.52	193/14520 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	X	0.0±0.0	0.2±0.5
All	All	0	7

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	X	152	THR	CB-CG2	-8.06	1.25	1.52	12	1
1	X	118	HIS	N-CA	-6.89	1.37	1.46	30	1
1	X	152	THR	N-CA	-6.69	1.38	1.46	12	1
1	X	143	ALA	CA-CB	-6.62	1.44	1.53	2	9
1	X	152	THR	CA-CB	5.90	1.60	1.52	6	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	X	150	LYS	N-CA-C	16.54	122.34	108.78	23	23
1	X	151	PHE	N-CA-C	13.64	130.28	109.96	22	30
1	X	130	GLY	N-CA-C	-9.81	94.88	110.18	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	X	152	THR	N-CA-CB	-8.37	98.10	110.24	12	1
1	X	143	ALA	N-CA-C	7.39	120.40	110.35	30	1
1	X	119	ARG	N-CA-C	7.35	119.29	111.28	22	1
1	X	136	GLY	N-CA-C	-7.34	105.66	115.21	11	25
1	X	153	CYS	N-CA-C	7.34	121.44	109.85	29	9
1	X	140	LEU	N-CA-C	-7.07	103.50	111.14	28	9
1	X	151	PHE	CB-CA-C	-6.91	100.20	110.16	22	2
1	X	164	ASP	N-CA-C	6.90	118.75	110.19	3	4
1	X	145	ARG	N-CA-C	6.51	119.44	107.99	19	11
1	X	130	GLY	CA-C-O	-6.39	114.51	121.48	26	5
1	X	150	LYS	CA-C-O	6.33	121.61	117.94	23	1
1	X	118	HIS	N-CA-C	6.24	119.66	110.30	5	1
1	X	145	ARG	CB-CA-C	-6.11	100.83	110.79	5	2
1	X	161	ILE	N-CA-C	6.01	115.91	107.37	17	1
1	X	163	LEU	N-CA-C	5.88	120.03	112.86	19	2
1	X	132	CYS	N-CA-C	-5.82	98.22	108.23	12	8
1	X	122	GLU	N-CA-C	5.66	118.40	109.96	10	3
1	X	154	HIS	N-CA-C	-5.62	102.70	110.35	12	2
1	X	122	GLU	CB-CA-C	-5.56	102.33	110.06	15	1
1	X	139	VAL	N-CA-C	5.53	112.13	106.21	18	3
1	X	118	HIS	CB-CA-C	-5.45	102.49	110.06	14	1
1	X	162	GLN	N-CA-C	5.29	117.80	111.71	30	3
1	X	151	PHE	N-CA-CB	-5.25	102.93	111.22	4	6
1	X	118	HIS	N-CA-CB	-5.22	100.72	109.28	30	1
1	X	165	CYS	N-CA-C	-5.17	99.78	110.80	26	1
1	X	154	HIS	N-CA-CB	5.17	117.64	109.83	29	1
1	X	154	HIS	CB-CA-C	-5.14	101.18	109.72	29	1
1	X	141	ARG	N-CA-C	-5.11	100.98	109.46	25	1
1	X	150	LYS	CA-C-N	5.08	128.54	121.02	22	1
1	X	150	LYS	C-N-CA	5.08	128.54	121.02	22	1
1	X	161	ILE	CB-CA-C	5.08	116.20	110.41	11	1
1	X	155	SER	N-CA-C	-5.01	105.82	111.28	24	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	X	156	GLU	Sidechain	3
1	X	164	ASP	Sidechain	2
1	X	122	GLU	Sidechain	2

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	X	357	345	345	3±1
All	All	10770	10350	10350	95

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:139:VAL:HG12	1:X:154:HIS:CD2	0.56	2.35	2	6
1:X:139:VAL:HG21	1:X:143:ALA:HB2	0.56	1.77	15	6
1:X:130:GLY:C	1:X:139:VAL:HG22	0.54	2.27	12	17
1:X:118:HIS:CD2	1:X:163:LEU:HA	0.51	2.40	19	2
1:X:166:ARG:HD2	1:X:166:ARG:H	0.48	1.69	14	1
1:X:145:ARG:HE	1:X:152:THR:HB	0.48	1.68	7	2
1:X:149:CYS:SG	1:X:165:CYS:HA	0.47	2.49	2	11
1:X:149:CYS:SG	1:X:150:LYS:N	0.46	2.88	12	11
1:X:135:CYS:HB3	1:X:137:ARG:HE	0.46	1.71	1	12
1:X:158:ARG:HD2	1:X:158:ARG:C	0.45	2.36	28	3
1:X:138:GLU:H	1:X:138:GLU:CD	0.44	2.20	7	1
1:X:150:LYS:HG3	1:X:151:PHE:H	0.44	1.73	21	1
1:X:166:ARG:HD2	1:X:166:ARG:C	0.44	2.38	22	1
1:X:166:ARG:HA	1:X:166:ARG:CZ	0.43	2.43	30	1
1:X:158:ARG:O	1:X:161:ILE:HG22	0.43	2.13	17	1
1:X:166:ARG:C	1:X:166:ARG:HE	0.43	2.22	19	2
1:X:145:ARG:HG2	1:X:152:THR:HB	0.42	1.90	6	4
1:X:118:HIS:HA	1:X:165:CYS:SG	0.42	2.55	20	2
1:X:118:HIS:HE2	1:X:161:ILE:HG21	0.42	1.74	26	1
1:X:118:HIS:HD2	1:X:120:PHE:CZ	0.41	2.33	22	1
1:X:118:HIS:HB2	1:X:120:PHE:CE2	0.41	2.51	20	3
1:X:141:ARG:HE	1:X:154:HIS:CD2	0.41	2.33	2	1
1:X:118:HIS:HA	1:X:146:CYS:SG	0.41	2.55	17	1
1:X:158:ARG:HD3	1:X:158:ARG:C	0.41	2.41	5	1
1:X:120:PHE:HB3	1:X:144:LEU:HB3	0.41	1.93	15	1
1:X:152:THR:O	1:X:152:THR:HG23	0.40	2.16	6	1
1:X:145:ARG:HD3	1:X:152:THR:HB	0.40	1.93	17	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	43/72 (60%)	38±1 (88±3%)	4±1 (9±3%)	2±1 (4±2%)	4	32
All	All	1290/2160 (60%)	1129 (88%)	115 (9%)	46 (4%)	4	32

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	X	149	CYS	24
1	X	164	ASP	9
1	X	150	LYS	4
1	X	118	HIS	3
1	X	162	GLN	3
1	X	147	ALA	1
1	X	163	LEU	1
1	X	129	PRO	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	40/62 (65%)	38±1 (96±3%)	2±1 (4±3%)	28	79
All	All	1200/1860 (65%)	1151 (96%)	49 (4%)	28	79

All 13 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	X	140	LEU	17
1	X	161	ILE	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	X	166	ARG	5
1	X	151	PHE	4
1	X	160	LEU	4
1	X	163	LEU	3
1	X	158	ARG	3
1	X	118	HIS	3
1	X	162	GLN	1
1	X	164	ASP	1
1	X	152	THR	1
1	X	150	LYS	1
1	X	141	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided